4 Cosserat Rods as Calculus of Variations Problems

In this Chapter we will discuss formulations of various rod boundary value problems as calculus of variations problems. We first in 4.1 restrict attention to the planar case, and consider the connections between various discrete and continuous problems. We describe both Lagrangian and Hamiltonian forms of the equilibrium conditions. Then in 4.2 we turn to the 3D case. After a parametrization of the group of $\mathbf{3} \times \mathbf{3}$ proper orthogonal matrices denoted $\boldsymbol{SO(3)}$ is introduced (we shall use the description known as *quaternions* or, more or less equivalently, *Euler parameters*) then the calculus of variations formulations for three dimensional rod deformations are immediately analogous to the planar cases.

Previously we have seen that when regarded as a finite difference approximation, the continuous limit of the first-order stationarity conditions for various planar, discrete, multiple-link strut problems yield the balance laws for moment when the only unknowns are angles, or for moment plus force when the unknowns are angles plus the cartesian coordinates of joints between the links. We also saw how various boundary conditions required either a global constraint (involving sums of the unknowns) or, for inextensible, unshearable models, link-wise constraints leading to multipliers associated with each link. In all cases we were able to make identifications with the analogous continuous equilibrium conditions via identification of the appropriate finite difference approximations.

The energies and constraints themselves also have finite difference limits, leading to various continuous calculus of variations problems of minimizing an appropriate energy with or without constraints of various types. With the general theory of the calculus of variations described in the last Chapter now in hand, we can proceed to derive the equilibrium conditions directly as Euler-Lagrange equations with various multiplier rules. The interesting consequence of this is that we can then work entirely within the context of a continuous Cosserat rod model of DNA, and still have the notion of stability, in the sense of whether or not a critical point is a local minimum. Moreover, although we do not examine the appropriate theory in detail, whether or not a stationary point is a local minimum (in an appropriate sense) can be readily computed via conjugate point tests associated with the second variation.

Having an entirely continuous model, including a variational principle, has various other beneficial features. First it frees us from the specific finite difference discretization that might be associated with a base-pair level description. This allows a separation between errors associated with numerics and errors associated with modelling (for example how to extract values for the $\hat{u}_i$ and stiffnesses from experimental data). It also allows the use of numerical discretizations that may be more suitable or convenient for various reasons, for example the adaptive collocation discretization used in AUTO that you have seen within the VBM software package. The calculus of variations formulation also reveals the appropriate route to deriving a Hamiltonian form of the equilibrium conditions, which in turn is important in the understanding of various symmetries and integrals which have an important impact on the physical problem.

However for our purposes in this course, the most important reason for deriving the relation between the planar discrete, and planar continuous variational formulations is that it makes it clear how to write down the calculus of variations formulations of 3D rod problems, while retaining the link with base pair level models and wedge angle data sets. In particular the utility of introducing a parametrization of the rotation group to describe the director frame is laid bare.

We proceed with a number of examples of various planar rod problems. The choice of examples directly parallels those for the discrete model described in Chapter 2, and comparison should be made to them. The examples also use and illustrate the general theory of the calculus of variations that was sketched in the previous chapter.

4.1 2d version

Example 1 (Moment balance for the planar inextensible, unshearable strut)

The continuous planar moment balance equation

$$-\big(K_2(s)(\phi'(s) - \hat{u}_2(s))\big)' - \lambda \sin\phi(s) = 0$$

is the Euler-Lagrange equation for the functional

$$\int_0^1 K_2(s)(\phi' - \hat{u}_2)^2/2 + \lambda \cos\phi \; ds.$$

Here we regard λ as a prescribed constant. With the parameter s being interpreted as arc-length (which is the same in both reference and deformed configurations because of inextensibility) the quadratic term in the integral can be recognized as the elastic strain-energy density for a planar inextensible, unshearable elastic rod with unstressed shape determined by $\hat{u}_2$, and a linear constitutive relation for bending with stiffness $K_2(s)$. For the strut boundary value problem we would have an imposed boundary condition only at $s = 0$, e.g.

$$\phi(0) = \alpha$$

so that the direction of the tangent to the centreline (or equivalently $\mathbf{d}_3(0)$) is prescribed at one end-point, and, following the conventions of our reduction to the planar case that were described in Chpt 2, the tangent is vertically upward when $\alpha = 0$.

Because there is no imposed boundary condition at $s = 1$ the natural boundary condition

$$K_2(1)(\phi'(1) - \hat{u}_2(1)) = 0$$

is one of the first-order necessary conditions. In this example the physical interpretation of the natural boundary condition is that the bending moment $m_2(1)$ vanishes, i.e. there is no moment applied to the end of the rod.

It also makes perfect sense to instead impose a boundary value for $\phi(1)$ say $\phi(1) = \beta$, in which case solutions to the Euler-Lagrange equation satisfying this boundary condition should be sought, and no natural boundary condition arises.

The physical interpretation of the term $\int_0^1 \lambda \cos\phi \; ds$ is a potential energy associated with a constant dead-loading (i.e. the load does not depend upon changes in the point at which it is applied) applied to the end point $s = 1$. The term could alternatively be written as $\lambda\, z(1)$ using the kinematic conditions

$$x'(s) = \sin\phi(s), \qquad z'(s) = \cos\phi(s)$$

which allow the centerline of the rod $(x(s),\, 0,\, z(s))$ to be reconstructed from knowledge of the tangent angle $\phi(s)$.

In the notational conventions introduced earlier $\lambda > 0$ corresponds to a load pushing down on the rod, i.e. to a load that is likely to produce buckling when sufficently large. Force balance is not implied by this variational principle, but rather has already been used to eliminate the variables $x(s)$ and $z(s)$, to reduce the energy to being a functional of the tangent angle ϕ only.

In the above (and also below) the particular (offset) quadratic strain-energy density function $K_2(s)(\phi' - \hat{u}_2)^2/2$ could be replaced with a general (offset) nonlinear function $W(\phi' - \hat{u}_2,\, s)$ that is convex in its first argument. The linear constitutive relation for bending

$$m_2(s) = K_2(s)(\phi'(s) - \hat{u}_2(s))$$

is merely replaced with the nonlinear constitutive relation

$$m_2(s) = W_{p_1}(\phi'(s) - \hat{u}_2(s), s)$$

where W_{p_1} denotes the partial derivative with respect to the first argument of W, and the Euler-Lagrange equation is modified to become

$$-\left(W_{p_1}(\phi'(s) - \hat{u}_2(s), s)\right)' - \lambda \sin\phi(s) = 0.$$

Example 2 (Boundary conditions on x and z expressed as isoperimetric constraints on ϕ)

Boundary conditions such as $x(0) = 0$ and $z(0) = 0$ are innocuous in establishing a variational principle for planar rod equilibria in terms of only the tangent angle ϕ, because they can be satisfied merely by choice of initial conditions when solving the kinematic ODE to reconstruct the centreline from the tangent angle. In fact there is no loss of generality in imposing the side conditions $x(0) = 0$ and $z(0) = 0$ because they merely eliminate the symmetry of translation in space (or equivalently prescribe an otherwise arbitrary choice of origin). However if there are *two* boundary conditions on x (or on z) a nonlinear isoperimetric constraint on ϕ is implied. For example if we are seeking solutions satisfying $x(1) - x(0) = \gamma$, then we should seek tangent angles satisfying the constraint

$$\int_0^1 \sin\phi \, ds = \gamma.$$

(The case $\gamma = 0$ would be the most usual.)

Then the variational principle for the planar equilibria is to minimize

$$\int_0^1 K_2(s)(\phi' - \hat{u}_2)^2/2 + \lambda \cos\phi \; ds.$$

subject to the isoperimetric constraint

$$\int_0^1 \sin\phi \, ds = \gamma,$$

and, say, the imposed boundary condition $\phi(0) = \alpha$. We therefore modify the functional to be made stationary by the addition of a (constant) Lagrange multiplier to obtain

$$\int_0^1 \left(K_2(s)(\phi' - \hat{u}_2)^2/2 + \lambda \cos\phi + \nu \sin\phi\right) \; ds,$$

(the sign convention associated with ν is arbitrary). The Euler-Lagrange equations are then

$$-\left(K_2(s)(\phi'(s)-\hat{u}_2(s))\right)' - \lambda \sin\phi(s) + \nu\cos\phi(s) = 0$$

where now the unknowns are the pair $(\phi(s), \nu)$ made up of the unknown function $\phi(s)$ and the unknown constant ν. The constant must be picked so that the corresponding solution $\phi(s)$ of the Euler-Lagrange equations satisfies the isoperimetric constraint.

The role of imposed and natural boundary conditions on $\phi(s)$ are exactly the same in the presence or absence of an isoperimetric constraint, because, in the above case, the isoperimetric constraint does not involve any derivatives of ϕ, so the integration by parts argument that leads to the natural boundary conditions is unaffected.

Comparison with the appropriate planar version of the coordinate free equilibrium equations

$$\mathbf{m}' + \mathbf{r}' \times \mathbf{n} = 0, \qquad \mathbf{n}' = 0$$

reveals that ν has the physical interpretation of being the unknown horizontal force of reaction of the boundary support, or horizontal end-load, that enforces the boundary condition $x(1) - x(0) = \gamma$. (The direction of the force corresponding to $\nu > 0$ depends upon the sign convention originally chosen.) This is in contrast to the parameter λ which we have so far interpreted as a *known* parameter that is specified beforehand and which gives the vertical component of the end load. In fact one could also consider problems where both $x(1) - x(0)$ and $z(1) - z(0)$ are specified, in which case both λ and ν would be undetermined Lagrange multipliers corresponding to the components of the unknown force required to maintain the boundary conditions. (One must be a little careful in this doubly constrained problem in formulating a well-posed problem—for example, if the rod is assumed inextensible of length 1, the specified distance between the two end-points must certainly be less than 1, or there can be no solution.) On the other hand one could specify both λ and ν to have given values, in which case both $x(1) - x(0)$ and $z(1) - z(0)$ are determined as part of the solution procedure. In point of fact the strut of Example 1 is precisely of this form, with $\nu = 0$ prescribed. The fact is that in a well-posed problem either the component of force or a component of displacement (or some combination of them) should be specified. The situation is analogous to the fact that in any calculus of variations problem for each component of an unknown function $\mathbf{w}(s)$ and at each end-point, there is either an imposed boundary condition (which should not involve the component of the derivative $\mathbf{w}'$) or a natural boundary condition (involving the component of the derivative $\mathbf{w}'$).

For inextensible unshearable rods the situation is clarified in the next example:

Example 3 (moment *and* force balance for inextensible, unshearable planar deformations)

In Examples 1 and 2 there was one basic unknown function, namely the tangent angle $\phi(s)$ and consequently there was one scalar Euler-Lagrange equation, which turned out to correspond to the moment balance for a planar rod, provided that it is *assumed* that the force balance $\mathbf{n}' = \mathbf{0}$ is satisfied. We now turn to a calculus of variations problem with three unknowns $\phi(s)$, $x(s)$, $z(s)$ whose three Euler-Lagrange equations are the single scalar moment balance, and the two components of force balance that arise for planar deformations.

It is now just as convenient to switch to a general nonlinear, convex strain energy density function $W(\phi'(s) - \hat{u}_2(s), s)$ for an inextensible, unshearable rod. Consider the following calculus of variations problem which involves pointwise constraints:

$$\int_0^1 W(\phi'(s) - \hat{u}_2(s), s)\, ds + \lambda z(1)$$

which is regarded as a functional depending on $\phi(s)$, $x(s)$, and $z(s)$, subject to the imposed boundary conditions

$$\phi(0) = 0, \qquad z(0) = 0, \qquad x(0) = 0, \qquad x(1) = 0$$

and subject to the pointwise constraints expressing inextensibility and unshearability

$$x'(s) = \sin\phi(s), \qquad z'(s) = \cos\phi(s).$$

Here the integral term is the strain energy associated with bending, and now the potential energy from the vertical dead loading at $s = 1$ is as expressed as the pointwise term $\lambda z(1)$. Because the functions $x(s)$, and $z(s)$ are basic unknowns in this formulation there is no need to re-write the boundary conditions on them in terms of one or more isoperimetric constraints on the tangent angle ϕ. Now however we must introduce two unknown functions $\mu_1(s)$ and $\mu_3(s)$ as unknown multiplier functions associated with the pointwise constraints. (The choice of numbering $\mu_1(s)$ and $\mu_3(s)$ is natural due to our embedding the planar problem into the (x, z) plane with $y = 0$.)

The modified Lagrangian so obtained is

$$\int_0^1 \left(W(\phi'(s) - \hat{u}_2(s), s) + \mu_1(s)(x'(s) - \sin\phi(s)) + \mu_3(s)(z'(s) - \cos\phi(s)) \right) \, ds + \lambda z(1)$$

with the three Euler-Lagrange equations (w.r.t. x, z and ϕ respectively) being

$$-\{\mu_1(s)\}' = 0 \tag{4.41}$$

$$-\{\mu_3(s)\}' = 0 \tag{4.42}$$

$$-\left(W_{p_1}(\phi'(s) - \hat{u}_2(s), s)\right)' - \mu_1(s)\cos\phi(s) + \mu_3(s)\sin\phi(s) = 0 \tag{4.43}$$

(4.44)

The first two equations are particularly simple because x and z only enter the problem linearly and only through the terms x' and z' appearing in the pointwise constraints. The first two equations can be recognized as force balance $\mathbf{n}' = \mathbf{0}$ with $\mathbf{n}(s) = (x(s), 0, z(s))$, or $\mathbf{n}$ constant $\mathbf{n} = (-\nu, 0, -\Lambda)$ for some constants ν and Λ. The undetermined constant ν representing the unknown horizontal component of the force $\mathbf{n}$ can be seen to be playing exactly the same role as the undetermined constant multiplier ν associated with the isoperimetric constraint in Example 2: the only difference is that in Example 2 the multiplier is associated with an isoperimetric constraint and is known *a priori* to be constant, whereas in the formulation of Example 3 the multiplier is associated with a pointwise constraint, is *a priori* a function of s and is only known to be constant because of the simple form of the associated Euler-Lagrange equations. The same structure that implies that the Euler-Lagrange equations in the formulation of Example 3 are simple, also implies that the problem can be formulated as in Example 2—that is the variables x and z appear in such a way that they are *ignorable*, which means that the problem can be reduced to one for the tangent angle ϕ alone, possibly with an isoperimetric constraint (or two) to express the vestige of boundary conditions on x and z.

From what we have seen thus far it is clear that the constants Λ and λ should be related to each other. How does this come about mathematically? It is through the natural boundary conditions. In this example there are imposed boundary conditions on all three unknown functions at $s = 0$ so at $s = 0$ all boundary terms arising from the integration by parts used in deriving the Euler-Lagrange vanish, and there are no associated natural boundary conditions. However at $s = 1$ there is the single imposed boundary condition $x(1) = 0$, so we can anticipate there being two natural boundary conditions. Explicitly the boundary terms that arise are

$$W_{p_1}\bar{\phi} + \mu_1\bar{x} + \mu_3\bar{z} + \lambda\bar{z}$$

Here all functions are to be evaluated at $s = 1$, $\bar{\phi}$, $\bar{x}$ and $\bar{z}$ denote the variations in the functions ϕ, x and z, and the term $\lambda\bar{z}$ arises from linearization of the pointwise term $\lambda\, z(1)$ appearing in the functional to be minimized. The sum of the boundary terms arising in the integration by parts of the first variation, must vanish for all allowed variations. Because of the imposed boundary condition on $x(1)$ we know $\bar{x}(1) = 0$ and that term drops out, but for allowed variations both $\bar{\phi}(1)$ and $\bar{z}(1)$ can either be non-zero or zero. Considering first $\bar{\phi}(1) \neq 0$ and $\bar{z}(1) = 0$, we can conclude that W_{p_1} evaluated at $s = 1$ must vanish, i.e. there is a natural boundary condition that the bending moment vanish. Then considering $\bar{z}(1) \neq 0$ we conclude that there is a second natural boundary condition namely that

$$\mu_3(1) + \lambda = 0$$

or

$$\lambda = -\mu_3(1) = -\Lambda$$

where as before Λ is the constant appearing in our integration of the Euler-Lagrange equations. Thus, as anticipated, the constants λ and Λ are both simply related to the vertical component of the boundary value of the force.

Example 4 (shearable extensible planar deformations)

For a shearable, extensible rod the problem is to minimize

$$\int_0^1 W(v_1 - \hat{v}_1(s),\, v_3 - \hat{v}_3(s),\, \phi'(s) - \hat{u}_2(s), s)\, ds + \lambda z(1)$$

subject to the imposed boundary conditions

$$\phi(0) = 0, \qquad z(0) = 0, \qquad x(0) = 0, \qquad x(1) = 0.$$

The functional is regarded as depending on the unknown functions $\phi(s)$, $x(s)$, and $z(s)$, with $\hat{v}_1(s)$, $\hat{v}_3(s)$ and $\hat{u}_2(s)$ being prescribed functions of s determining the unstressed shape, and with v_1 and v_3 being place holders defined through

$$v_1 = x' \cos\phi - z' \sin\phi \tag{4.45}$$

$$v_3 = x' \sin\phi + z' \cos\phi \tag{4.46}$$

This specific notation is consistent with the general one introduced for extensible shearable 3D Cosserat rods once it is recognized that in the specific reduction from 3D to 2D introduced earlier

$$\mathbf{d_1} = (\cos\phi,\ 0,\ -\sin\phi) \tag{4.47}$$
$$\mathbf{d_3} = (\sin\phi,\ 0,\ \cos\phi) \tag{4.48}$$
$$\mathbf{r}' = (x',\ 0,\ z') \tag{4.49}$$
$$v_1 = \mathbf{r}'\cdot\mathbf{d_1} \tag{4.50}$$
$$v_3 = \mathbf{r}'\cdot\mathbf{d_3} \tag{4.51}$$
$$u_2 = \phi' \tag{4.52}$$

The variational principle involves a standard Lagrangian $L(s,\phi,x,z,\phi',x',z')$ that is explicitly defined through a composition of the given strain energy density function $W(v_1 - \hat{v}_1(s),\ v_3 - \hat{v}_3(s),\ u_2 - \hat{u}_2(s), s)$ with the interpretations of v_1 v_3 and u_2 appropriate for planar deformations in terms of the unknown functions $(\phi, x, z, \phi', x', z')$ that are given above.

We may therefore immediately compute the three Euler-Lagrange equations with respect to x z and ϕ, using the chain rule for differentiation:

$$-\frac{d}{ds}\left(W_{v_1}\cos\phi + W_{v_3}\sin\phi\right) = 0 \tag{4.53}$$
$$-\frac{d}{ds}\left(-W_{v_1}\sin\phi + W_{v_3}\cos\phi\right) = 0 \tag{4.54}$$
$$-\frac{d}{ds}\left(W_{u_2}\right) + W_{v_1}\left(-x'\sin\phi - z'\cos\phi\right) + W_{v_3}\left(x'\cos\phi - z'\sin\phi\right) = 0 \tag{4.55}$$

These equations have a direct physical interpretation. Recall that for a hyper-elastic rod the constitutive relations are given in terms of derivatives of the strain-energy density function

$$m_i = W_{u_i} \qquad n_i = W_{v_i}$$

where it should also be recalled that the m_i and n_i are components with respect to the variable director frame. For the planar deformations under consideration here, the director frame is completely specified by the single angle ϕ, and the first two Euler-Lagrange equations can be rewritten as

$$-\frac{d}{ds}\left(n_1\cos\phi + n_3\sin\phi\right) = -\frac{d}{ds}n_x = 0 \tag{4.56}$$
$$-\frac{d}{ds}\left(-n_1\sin\phi + n_3\cos\phi\right) = -\frac{d}{ds}n_z = 0 \tag{4.57}$$

where n_x and n_z denote the x and z components with respect to the fixed reference frame basis. Thus the first two Euler-Lagrange equations simply express the two planar components of the force balance equation $\mathbf{n}' = \mathbf{0}$, and take their simplest form when re-written with respect to the fixed frame.

Similarly the third Euler-Lagrange equation can be re-written in the form

$$-\frac{d}{ds}(W_{u_2}) - W_{v_1}v_3 + W_{v_3}v_1 = 0$$

which can be recognized as the y or 2 component of the moment balance equation $\mathbf{m}' + \mathbf{r}' \times \mathbf{n} = \mathbf{0}$ (with the other two components being identically satisfied for planar deformations of the form described above, and for appropriate 3D constitutive relations, see below)

Example 1' (Hamiltonian form of Euler-Lagrange equations in Example 1)

This is a standard application of the Legendre transform. The partial derivative of the functional

$$\int_0^1 K_2(s)(\phi' - \hat{u}_2)^2/2 + \lambda\cos\phi\, ds.$$

with respect to the derivative variable ϕ' reveals that the conjugate variable is

$$m_2 \equiv K_2(s)(\phi'(s) - \hat{u}_2(s))$$

which is equivalent to the constitutive relation defining the bending moment $m - 2$. The constituive relation or definiton of the conjugate variable can be inverted to give ϕ' in terms of the other variables

$$\phi' = m_2/K_2(s) + \hat{u}_2(s)$$

and the single second order equation

$$-\left(K_2(s)(\phi'(s) - \hat{u}_2(s))\right)' - \lambda\sin\phi(s) = 0$$

can be re-written as the system

$$\phi' = m_2/K_2(s) + \hat{u}_2(s) \tag{4.58}$$
$$m_2' = -\lambda\sin\phi \tag{4.59}$$

which is a one degree of freedom Hamiltonian system with Hamiltonian

$$m_2^2/K_2(s) + \hat{u}_2(s)m_2 - \lambda\cos\phi$$

where $K_2(s) > 0$ and $u_2(s)$ are given functions of s, λ is a given constant, and the problem is to find solutions satisfying the two point boundary value problem involving the imposed boundary condition $\phi(0)\alpha$ and the natural boundary condition $m - 2(1) = 0$.

In the case where the strain energy density function $W(\phi' - \hat{u}_2, s)$ is more general than quadratic, then it is usually the case that the definition

$$m_2 = W_{p_1}(\phi'(s) - \hat{u}_2(s), s)$$

cannot be explicitly inverted for the variable ϕ', However the conjugate variable can still be seen to be the bending moment defined by the appapriate constitutive relation, and by the assumed convexity of W it is known that there is some function Ψ such that

$$\phi' = \Psi(m_2, s) + \hat{u}_2(s).$$

Moreover

$$\Psi(p, s) = W^*_p(p, s)$$

where $W^*(p, s)$ is the Fenchel transform of the strain-energy function $W(q, s)$. Thus if the Fenchel transform $W^*(p, s)$ of the strain-energy function $W(q, s)$ is regarded as known, then the Euler-Lagrange equations can be seen to be equivalent to the Hamiltonian system with Hamiltonian

$$W^*(m_2, s) + \hat{u}_2(s)m_2 - \lambda \cos \phi.$$

Example 2' (Boundary conditions on x and z expressed as isoperimetric constraints on ϕ)

This example is essentially the same as Example 1'. One derives a Hamiltonian system with Hamiltonian

$$W^*(m_2, s) + \hat{u}_2(s)m_2 - \lambda \cos \phi - \nu \sin \phi.$$

involving the additional unknown constant ν and the value of the constant must be picked so that the solution satisfying the appropriate boundary conditions also satisfies the integral side condition expressing the isoperimetric constraint.

Example 3' (Hamiltonian form in the presence of pointwise constraints of inextensibility and unshearability)

This problem is somewhat non-standard from the Hamiltonian point of view, and the necessary general theory (Dirac's theory of constraints combined with something called the impetus-striction formulation) is beyond the scope of the course. However the particular example can be understood in its own right, and provided that the motivation for why the example works the way it does, is set aside and regarded as a little black magic, things are quite straightforward.

The difficulty is that the effective Lagrangian, i.e. the Lagrangian including the multipliers $\mu_1(s)$ and $\mu_3(s)$ associated with the pointwise constraints

$$x'(s) = \sin\phi(s), \qquad z'(s) = \cos\phi(s),$$

is

$$\int_0^1 \big(W(\phi'(s) - \hat{u}_2(s), s) + \mu_1(s)(x'(s) - \sin\phi(s)) + \mu_3(s)(z'(s) - \cos\phi(s))\big)\, ds + \lambda z(1),$$

which is a strictly convex function of ϕ' (by assumption on the form of W), but is *not* a strictly convex function of x' and z' (it is clearly a linear function of x' and z'). When the standard prescription is followed and the conjugate variables are introduced by taking partial derivatives of the Lagrangian w.r.t. ϕ', x' and z' respectively we find

$$m_2 = W_{p_1}(\phi'(s) - \hat{u}_2(s), s) \tag{4.60}$$

$$n_x = \mu_1(s) \tag{4.61}$$

$$n_y = \mu_3(s) \tag{4.62}$$

(where we have prejudiced notation because of our physical based knowledge of the system). The problem comes because while we can solve the above for the variable ϕ' (just as we did in the previous examples because the system decouples) we cannot invert these relations to solve for x' and z' because they do not appear at all! The saving grace is that the constraints already give expressions for x' and z' in terms of the configuration variables (ϕ, x and z). (In fact only in terms of $\sin\phi$ and $\cos\phi$ but that is just an added simplification.) Therefore, if we set aside how the Hamiltonian was constructed, we can merely verify that the three degree of freedom Hamiltonian

$$W^*(m_2, s) + \hat{u}_2(s)m_2 + n_x \sin\phi + n_z \cos\phi$$

has associated Hamiltonian equations

$$\phi' = \Phi(m_2, s) + \hat{u}_2(s) \tag{4.63}$$
$$\mathrm{x}' = \sin\phi \tag{4.64}$$
$$\mathrm{z}' = \cos\phi \tag{4.65}$$
$$m_2' = -\lambda \sin\phi \tag{4.66}$$
$$n_x' = 0 \tag{4.67}$$
$$n_z' = 0 \tag{4.68}$$

which form a first-order system equivalent to the moment and force balance laws plus the constraints.

Example 4' (Hamiltonian form of equations for shearable extensible planar deformations)

As in Examples 1 and 1', Example 4' is again a straightforward application of the Legendre transform to pass from the Lagrangian second-order side of Example 4, to the Hamiltonian first-order side, except now there are three unknown functions $\phi(s)$, $x(s)$, and $z(s)$ and we anticipate a three degree of freedom Hamiltonian system. The only non-standard feature is that the 'Lagrangian' is defined as a composition of the function W with the functions v_1 and v_3 that are place holders as introduced in Example 4. Thus because W is not explicitly known, the standard formula for passing to the Hamiltonian must be applied using a chain rule and the Fenchel transform W^* of W and its properties.

Introducing the conjugate variables in the usual way leads to the equations

$$n_x = W_{v_1} \cos\phi + W_{v_3} \sin\phi \tag{4.69}$$
$$n_z = -W_{v_1} \sin\phi + W_{v_3} \cos\phi \tag{4.70}$$
$$m_2 = W_{u_2} \tag{4.71}$$

The first step is to invert these equations to solve for ϕ', x', and z'. This is actually easy once rotations and change of basis are recognized and exploited appropriately. First the right hand side should be identified as a simple rotation of the gradient of W through an angle $\phi(s)$ for each s. Inverting the rotation (i.e. multiplying by the transpose of the appropriate matrix) leads to the identities

$$W_{v_1} = n_x \cos\phi - n_z \sin\phi = n_1 \tag{4.72}$$
$$W_{v_3} = n_x \sin\phi + n_z \cos\phi = n_3 \tag{4.73}$$
$$m_2 = W_{u_2} \tag{4.74}$$

These equations are exactly inverted through the properties of the Fenchel transform $\boldsymbol{W}^*$ of $\boldsymbol{W}$ to obtain

$$\boldsymbol{v_1} - \boldsymbol{\hat{v}_1} = \boldsymbol{W}^*_{\boldsymbol{n_1}} \tag{4.75}$$

$$\boldsymbol{v_3} - \boldsymbol{\hat{v}_3} = \boldsymbol{W}^*_{\boldsymbol{n_3}} \tag{4.76}$$

$$\boldsymbol{u_2} - \boldsymbol{\hat{u}_2} = \boldsymbol{W}^*_{\boldsymbol{m_2}} \tag{4.77}$$

Here $\boldsymbol{W}^*$ is regarded as a known function of the variables $(\boldsymbol{n_1}, \boldsymbol{n_3}, \boldsymbol{m_2}, \boldsymbol{s})$ and therefore also a known function of the variables $(\boldsymbol{\phi}, \boldsymbol{n_x}, \boldsymbol{n_z}, \boldsymbol{m_2}, \boldsymbol{s})$ through composition with a simple rotation.

The next step is to solve for the variables $(\boldsymbol{\phi'}, \boldsymbol{x'}, \boldsymbol{z'})$, which is again straightforward because $\boldsymbol{\phi'} = \boldsymbol{u_2}$ and, from the kinematics summarized in Example 4, $(\boldsymbol{x'}, \boldsymbol{z'})$ are a rotation of $(\boldsymbol{v_1}, \boldsymbol{v_3})$ again through an angle $\boldsymbol{\phi(s)}$. We thus find that the inversion is complete with

$$\boldsymbol{x'} = (\boldsymbol{\hat{v}_1} + \boldsymbol{W}^*_{\boldsymbol{n_1}}) \cos\boldsymbol{\phi} + (\boldsymbol{\hat{v}_3} + \boldsymbol{W}^*_{\boldsymbol{n_3}}) \sin\boldsymbol{\phi} \tag{4.78}$$

$$\boldsymbol{z'} = -(\boldsymbol{\hat{v}_1} + \boldsymbol{W}^*_{\boldsymbol{n_1}}) \sin\boldsymbol{\phi} + (\boldsymbol{\hat{v}_3} + \boldsymbol{W}^*_{\boldsymbol{n_3}}) \cos\boldsymbol{\phi} \tag{4.79}$$

$$\boldsymbol{\phi'} = \boldsymbol{\hat{u}_2} + \boldsymbol{W}^*_{\boldsymbol{m_2}} \tag{4.80}$$

We are now in a position to explicitly carry out the Legendre transform. The point of this example is that the rotation involved in the definition of the energy as $\boldsymbol{W}$ of a rotated variable exactly cancels with the rotation introduced in the inversion above, and the Hamiltonian is given by the expression

$$\boldsymbol{H}(\boldsymbol{\phi}, \boldsymbol{m_2}, \boldsymbol{n_x}, \boldsymbol{n_z}, \boldsymbol{s}) = \boldsymbol{W}^*(\boldsymbol{n_1}, \boldsymbol{n_3}, \boldsymbol{m_2}, \boldsymbol{s}) + \boldsymbol{n_1}\boldsymbol{\hat{v}_1} + \boldsymbol{n_3}\boldsymbol{\hat{v}_3} + \boldsymbol{m_2}\boldsymbol{\hat{u}_2}$$

where the right hand side is a composition with $\boldsymbol{W}^*(\boldsymbol{n_1}, \boldsymbol{n_3}, \boldsymbol{m_2}, \boldsymbol{s})$ assumed given, and $(\boldsymbol{n_1}, \boldsymbol{n_3})$ placeholders for functions of $(\boldsymbol{n_x}, \boldsymbol{n_z}, \boldsymbol{\phi})$ that are defined through the rotation

$$\boldsymbol{n_1} = \boldsymbol{n_x} \cos\boldsymbol{\phi} - \boldsymbol{n_z} \sin\boldsymbol{\phi} \tag{4.81}$$

$$\boldsymbol{n_3} = \boldsymbol{n_x} \sin\boldsymbol{\phi} + \boldsymbol{n_z} \cos\boldsymbol{\phi} \tag{4.82}$$

4.2 3d version

Here use a new Hamiltonian formulation of rod equilibrium conditions that exploits the Euler parameter description of $\boldsymbol{SO(3)}$ to determine the directors $\mathbf{d}_i(\boldsymbol{s})$.

A set of Euler parameters is a quadruple of real numbers

$$\mathbf{q} = (q_1, q_2, q_3, q_4)$$

that satisfies the identity

$$\mathbf{q} \cdot \mathbf{q} = {q_1}^2 + {q_2}^2 + {q_3}^2 + q_4^2 = 1 \ .$$

In other words a set of Euler parameters, or *unit quaternion*, is an element of the unit sphere $\mathbf{S}^3$ in $\Re^4$.

The components of the orthonormal triad $\{\mathbf{d}_i\}$ (with respect to the fixed space basis) are quadratic functions of the Euler parameters $\mathbf{q}$, e.g.

$$\mathbf{d}_3 = \begin{pmatrix} 2(q_1 q_3 + q_2 q_4) \\ 2(q_2 q_3 - q_1 q_4) \\ -q_1^2 - q_2^2 + q_3^2 + q_4^2 \end{pmatrix} .$$

Euler parameters (or quaternions) have the property that there exist three 4×4 skew-symmetric matrices $\mathbf{B}_i$ with entries 0 or ± 1 with the property that for any $\mathbf{q}$, $\{\mathbf{q}, \mathbf{B}_i \mathbf{q}\}$ forms an orthonormal basis of $\Re^4$.

Moreover

$$u_i = 2\mathbf{q}' \cdot \mathbf{B}_i \mathbf{q} / |\mathbf{q}|^2$$

Implies energy is convex but not strictly convex function of $\mathbf{q}'$.

In the Hamiltonian formulation the force $\mathbf{n}$ is the variable conjugate to the centerline $\mathbf{r}$.

And the Euler parameters $\mathbf{q}$ are conjugate to (the mystery variable) μ, which is more or less equivalent to the three director components of the moment $\mathbf{m}$. In terms of $\mathbf{z} = (\mathbf{x}, \mathbf{q}, \mathbf{n}, \mu) \in \Re^{14}$ the equilibrium and kinematic conditions reduce to a 7 degree of freedom Hamiltonian system (i.e. 14 first order ODE)

$$\mathbf{z}' = \mathcal{J} \nabla H(\mathbf{z})$$

where $\mathcal{J}$ is the canonical skew matrix

$$\mathcal{J} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

For a linear constitutive law the Hamiltonian $H(\mathbf{z})$ is

$$\mathbf{n} \cdot \mathbf{d}_3 + \frac{1}{2} \sum_i \left\{ m_i(s)^2 / K_i(s) + \hat{u}_i m_i \right\}$$

where the $\hat{\boldsymbol{u}}_i$ are the strains of the unstressed state, and the components of bending moment are written in terms of the phase variables by:

$$m_i = \frac{\boldsymbol{\mu} \cdot \mathbf{B}_i \mathbf{q}}{2} \qquad i = 1, 2, 3.$$

Thus the Hamiltonian is a quartic polynomial of the unknowns. Note that the Hamiltonian is a convex but not strictly convex function of $\boldsymbol{\mu}$. The Hamiltonian system always has eight integrals, five of which are in involution. Ten integrals, seven of which are in involution are obtained when the rod is uniform and isotropic. In the linearly elastic case this means $\boldsymbol{K}_1 = \boldsymbol{K}_2$ with both constant, and $\hat{\boldsymbol{u}}_1 \equiv \hat{\boldsymbol{u}}_2 \equiv \mathbf{0}$.

Seven integrals in involution is classic condition for complete integrability of a Hamiltonian system. Means that in principle the initial value problem can be solved by quadrature. For this rod model can actually solve in closed form—goes back to Landau and Lifschitz, Illyukin, and more recently rediscoverd by Langer and Singer and by Shi and Hearst.

Unfortunately solution by quadrature has unknown constants that must be picked to yield correct solution to a two-point boundary value problem. Very intractable and numerically ill-conditioned problem. Much more efficient numerically to compute from scratch. Particularly because in non-integrable cases there is no other choice.

As a consequence of the exploitation of Euler parameters, all but one of the integrals are quadratic functions of the phase variables. Combines very well with numerics based on Gaussian collocation which is equivalent to a symplectic Runge-Kutta method that exactly conserves quadratic invariants.

In two point boundary value problems integrals 'convect' information from one end point to the other.

This is the key point in our techniques for the elimination of continuous symmetries that then allows numerically efficient parameter continuation.

We consider the boundary value problem corresponding to a closed twisted ring, with configurations of 'DNA' loops with different links arising when the angle parameter increases through multiples of 2π.

Numerical continuation requires a known solution as a starting point. For this rod BVP, explicit solutions only arise in the case of uniform isotropy.

We shall use the solution set for the uniformly isotropic loop as an organizing center for computation in the general case.

The associated 'perfect' bifurcation diagram has one intricately connected component — highly desirable for the continuation methods we employ.

Connectivity is forced by the (continuous) symmetries that are present. Same symmetries imply that each equilibrium is non-isolated (for fixed loading parameter)—very bad for standard continuation methods. Have to be careful to get round this, and solve a modified BVP that selects isolated representatives of symmetry generated families of equilibria.

Use Hamiltonian form of the equations and the integrals associated with the symmetries to modify the boundary conditions in such a way that efficient numerical continuation can be employed.

Add boundary conditions to factor out symmetries. An overdetermined system arises with more boundary conditions than equations. Standard numerical continuation packages (in our case AUTO) cannot handle this.

General idea for systems of Euler-Lagrange Equations with symmetry:

Symmetries generate non-isolation, that necessitate the addition of boundary conditions. With Hamiltonian structure, the same symmetries also generate integrals (Noether's Theorem). Use the integrals to show that some of the original boundary conditions are actually implied and need not be enforced.

Approach works beautifully in the rod problem. Analytically reduce to a formally well-posed system with equal numbers of boundary conditions and equations. AUTO is then very happy.

Breaking symmetries becomes delicate, for boundary conditions must be changed. Numerics are rather robust, and perform very well. Perhaps (probably?) associated with exact invariance of quadratic integrals provided by collocation techniques.

For the closed, twisted loop, an appropriate set of fourteen boundary conditions is

$$\mathbf{r}(0) = \mathbf{r}(1) = (0,\, 0,\, 0)$$

$$(q_1(0),\, q_2(0),\, q_3(0)) = (0,\, 0,\, 0)$$

$$\begin{aligned}(q_1(1),\, q_2(1),\, q_3(1), q_4(1))\\ &= (0,\, 0,\, -\sin(\theta/2),\, -\cos(\theta/2))\end{aligned}$$

$$\mu_4(0) = 0$$

But these boundary conditions have nonisolated equilibria for a uniformly isotropic rod.

14 boundary conditions leading to isolated equilibria for the integrable rod:

$$\mathbf{r}(0) = \mathbf{r}(1) = (0,\ 0,\ 0)$$

$$(q_1(0),\ q_2(0),\ q_3(0)) = (0,\ 0,\ 0)$$

$$q_3(1) = -\sin(\theta/2), \quad q_4(1) = -\cos(\theta/2),$$

$$\mu_4(0) = 0, \quad n_2(0) = 0, \quad n_3(0) = 0$$

The direction of the force $\mathbf{n}$ is fixed, but the values of $q_1(1)$ and $q_2(1)$ are not prescribed, which is equivalent to not requiring $\mathbf{d}_3(0) = \mathbf{d}_3(1)$. Using integrals of the system it can be shown that these boundary conditions are actually implied by the others. (At least locally.)

The boundary value problem for uniformly isotropic rods has closed form solutions comprising N-covered circles with uniform twist. Actually two sets of families, one with positive twist, and one with negative twist.

Each family of N-covered circles has a countable sequence of bifurcation points indexed by M say.

Numerics indicate that the branch emanating from the Mth bifurcation on the N-covered ring with positive twist links to the Nth bifurcation point on the M-covered ring with negative twist. Symbolically

$$(M, N, +) \leftrightarrow (N, M, -)$$